

2016 ASMS Workshop Report

FTMS: Day-to-Day Concerns for High Resolution Mass Analysis

Wednesday June 8, 2016: 5:45-7:00 pm

Don Smith and David Kilgour, Presiding

Estimated Attendance: 100

Summary of Program and Discussion

The aim of the workshop was to discuss the highest priorities for further development of FT-MS instrument capability. In order to help guide discussions, a poll was sent to the FTMS interest group prior to the workshop, however the results were ambiguous, so the workshop began with a re-polling the attendees concerns regarding future FTMS developments. The results of the poll are shown in **Figure 1**.

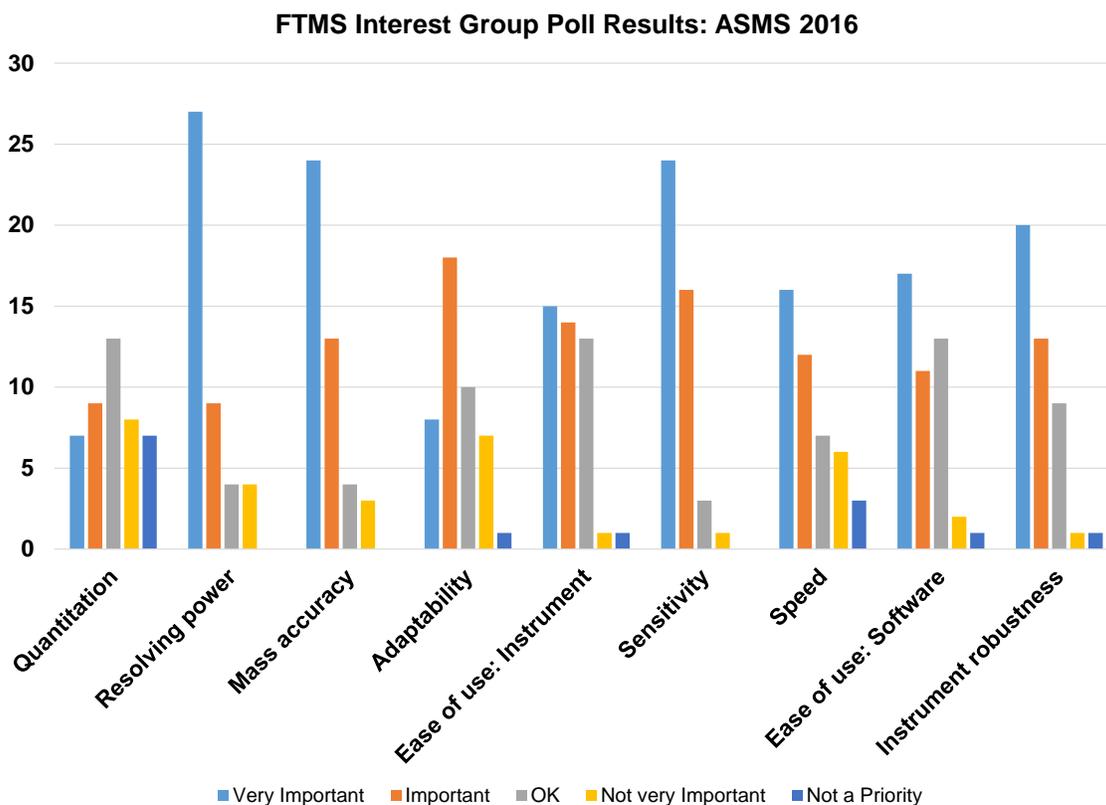


Figure 1: Results from 2016 ASMS FTMS interest group poll on which aspects of FTMS are most important to the community.

During the workshop, discussion points were collected using a Padlet. Padlet is website hosting virtual whiteboards/noticeboards that allow people to express and organize their collective thoughts on a common topic easily. Participants could post to the FTMS workshop Padlet, during the meeting, using web-browsers or apps on their smart phones, tablets or laptops; or by asking the chairs to post on their behalf. The Padlet produced during the workshop is shown in **Figure 2**.

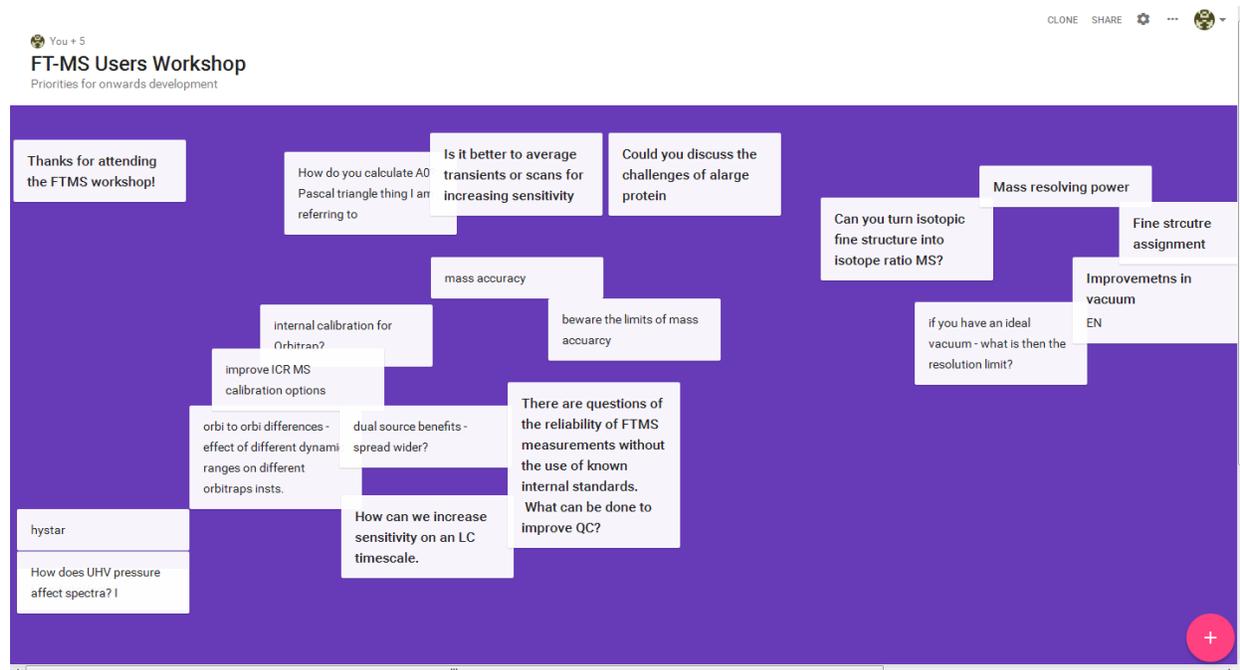


Figure 2: Padlet from open discussion at the 2016 ASMS FTMS workshop.

The results of the survey indicated that the user community stresses resolving power, mass accuracy and sensitivity as their highest priorities – so these formed the core of the discussion. Care was taken to separate out the different concerns of the three different communities within the FT-MS sphere: FT-ICR, Orbitrap and other FT-MS instrumentation.

Within the topic of mass resolving power, discussions included a desire for the increased availability of the use of isotopic fine structure for molecular formula confirmation, and concerns were raised regarding the adequacy of the ultra-high vacuum of commercial FT-ICR mass spectrometers (and FT-MS instruments more broadly) and the limitations this imposes on resolution.

Mass measurement accuracy was heavily discussed; concerns were raised regarding how commercial vendors are performing mass calibration in their software, and if there could be more options, using more advanced calibration methods in the future. The discussion included abundance correction calibration, internal calibration for Orbitrap mass spectrometers (including lock mass), performance variations between nominally similar Orbitrap systems, FT-ICR MS calibrations for MS imaging, the use of proper calibrants for different analytes of interest, and the use of dual ionization sources for injection of internal calibrants.

Sensitivity discussions included concerns regarding the underlying methods by which Thermo instrument calculate signal-to-noise ratio, and the difference between averaging time domain transients (μ scans on Thermo) and spectral averaging (scans).

An announcement was made that a replacement for Don Smith was needed, and the workshop was adjourned.